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Mechanisms of direct detonation initiation via thermal explosion of radiatively heated gas-particles layer

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ABSTRACT

Conceptual approach of detonation wave direct initiation by external radiative heating of microparticles locally suspended in flammable gaseous mixture is proposed. Combustion waves and detonation initiation mechanisms in the congestion regions of microparticles heated by radiation are studied numerically. Necessary criteria on geometrical scales of gas-particles layer and spatial uniformity of particles distribution for successful detonation initiation are formulated.

Introduction

For at least 150 years volumetric gas–vapor and dust explosions were of paramount interest because of their hazardous potential for industry including chemical plants, coal mines, nuclear power plants, gaseous storages, electric and optical cable ducts etc. On the other hand nowadays the interest to effective regimes of gaseous combustion is stimulated by the possibilities of using gaseous fuels in contemporary and perspective engines. Thus, for example, in propulsion systems design it is promising to use detonative regime [1,2] instead of deflagration (slow combustion).

To solve both problems of safety and efficient utilization of gaseous combustion energy one should determine the basic features of combustion evolution in the conditions corresponding to the scenarios interesting from a practical point of view. To solve that kind of coupled task one usually considers the combustion wave development out from the localized ignition kernel. The basic mechanism of such a combustion wave formation is a thermal explosion inside the kernel. Evolution of thermal explosion and eventual combustion regime are fully determined by the features of energy input. In the simplest case of volumetric thermal energy input everything is determined by the energy source spatial localization, its power and amount of input energy [3]. In reality physicochemical effects intrinsic to the nature of energy source (electric discharge, laser spark, shock wave etc.) are crucial and should be taken into account. The most deterministic and easily described is ignition by the heated surface. Thermal wave forms a heated kernel in the vicinity of the surface that leads to the ignition. A small spatial scale of the ignition kernel is the main disadvantage of this approach. Ignition kernels of such sizes are unable to ignite a detonation and could be strongly disturbed by the external flows.

In case of a closed insulated vessel with thick walls it is possible to create conditions for volumetric explosion of the gaseous mixture by slow quasi equilibrium heating. Needless to say that in this case one faces a challenge of utilization of the combustion energy released in that way. Another opportunity to get volumetric explosion inside closed vessel is a fast compression by the piston. The released energy acts against the piston action that is essential principle of perspective HCCI engines development. One more opportunity based on volumetric heating of the gas by the hot suspended particles can be proposed. As the gas is almost transparent for a wide spectrum of radiation the particles can be heated distantly by means of thermal or laser radiation. For the first time such a mechanism was examined in connection with explosion safety problems [4,5]. One of the most interesting scenarios among those considered was a severe accidental explosion inside the optical cable duct. It was concluded that particles suspended in the explosive gaseous atmosphere can cause its ignition when laser radiation is delivered by optical fibers. In [5,6] the ignition by the single sub-millimeter or micron size heated particle was studied. In [7,8] the ignition by the heated particles layers was considered. As the layer comprises a large amount of volumetrically suspended micro-particles it acts on a gas as a volumetric source of thermal energy. Every particle transfers the excess thermal energy from its surface to the surrounding gas and as a result a spatial

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temperature distribution establishes inside the gaseous phase. In case of reactive particles the additional energy and vapor products release causes higher temperatures inside the heated layers. Large amounts of excess energy occur to be carried by the dense carbon compounds like nano-diamonds, graphite and nano-tubes. Relatively low activation energy of such a compounds (~650 K) provides an opportunity to use rather low-power light sources for efficient volumetric heating of the gaseous mixture [9] and even triggering of detonation [10].

While studying the phenomena related with gaseous ignition by the radiatively heated particles [4,7] it was assumed that hot combustion products irradiate with sufficient intensity. Recently [11] such a scenario was considered and confirmed numerically. It was shown that a distant thick cloud of reactive gas with suspended inactive micro particles can be ignited in either deflagrative or detonative regime. On the basis of available experimental data and our recent calculations a conceptual approach for spatially localized direct combustion or detonation initiation can be proposed. Such an approach could be of primal interest for propulsion means, where fixed spatial-time scales of ignition and directed impulse are desired. The aim of this paper is to substantiate the suggested approach of localized thermal explosion via the radiative heating of the suspended microparticles. We consider possible scenarios of ignition kernels formation and resultant combustion regimes evolution in the localized volume of gaseous combustible mixture with suspended microparticles under effect of the external radiative energy source. Sensitivity of the developing combustion regimes toward particles spatial distribution and energy source intensity is studied. It allows us to formulate criteria for proposed concept applicability. The analysis is carried out by means of numerical simulations for hydrogen–oxygen gaseous combustible mixture.

Problem setup

To formulate a problem setup and mathematical model first let us introduce parameters determining the gaseous medium with volumetrically suspended microparticles. The state of gaseous mixture is characterized by mass density ρ, temperature T, pressure p, mass fractions of gaseous species Y_k, specific internal energy can be calculated as $\varepsilon = c_V T + \sum_k h_k Y_k$, where c_V is specific heat capacity at constant volume and h_k is enthalpy of formation of k species. Dispersed phase of suspended microparticles is characterized by mean diameter of the particles d_p assuming their spherical shape, material density ρ_{p0}, mean particles mass calculated as $m_p = \rho_{p0} V_p$, where V_p is a volume of spherical particle of given diameter d_p, specific heat capacity at constant pressure $c_{P,p}$, temperature T_p, particles number density N_p, mass density $\rho_p = m_p N_p$ and volume fraction $\alpha_p = \rho_p/\rho_{p0}$. Taking into account that the gaseous phase is almost transparent for radiation the mean free path of radiation inside the gas-particle layer of certain parameters can be estimated as:

$$\Lambda = 4\left(\pi d_p^2 N_p\right)^{-1} \tag{1}$$

or $\Lambda = 2d_p/3\alpha_p$. Within considered model it was also assumed that combustion products remained transparent for the radiation.

Assume the following problem setup represented in Fig. 1. The infinite planar channel filled with stoichiometric hydrogen–oxygen mixture at normal conditions (300.0 K and 1.0 bar). The layer of thickness L_1 carries uniformly suspended inactive microparticles. The referential parameters of suspended particles are following: diameter $d_p = 1.0$ μm, material density $\rho_{p0} = 1.0$ g/cm^3, specific heat capacity $c_{P,p} = 107$ erg/g/K, volume fraction of the particles $\alpha_p = 1.0 \cdot 10^{-5}$–$4.0 \cdot 10^{-5}$. At this setup the mean free path of the radiation inside the layer can be estimated as $\Lambda = 6.7$–1.7 cm.

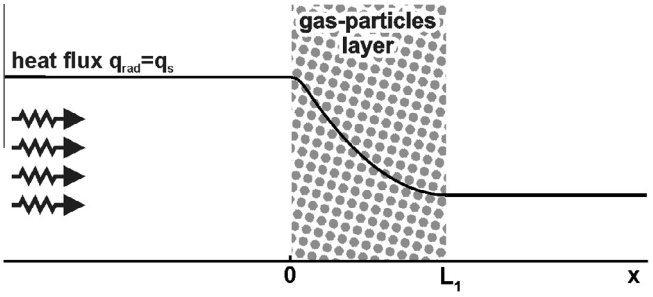

Fig. 1. Problem setup.

Constant blackbody heat flux is irradiated from the left end surface of the channel ($x \to -\infty$). It is assumed that radiative heat flux is instantly switched on at time $t = 0$. Parameters of the radiative energy source are the same as in [9,10]. The emitted heat flux $q_s = \sigma T^4$ corresponds to the blackbody surface with a temperature of 5800.0 K. In most of calculations the duration of the source action was not limited, it was found that in a number of cases radiation from the source together with hot combustion products radiation affected the thermal explosion evolution inside the gas-particles layer and had no influence on combustion after its formation in the cold gaseous medium. Therefore the obtained results also can be considered as the estimation of minimal radiative pulse duration required to ignite given combustion regime.

Numerical simulations were carried out in one-dimensional approximation using thoroughly tested reactive gasdynamics codes for calculating planar and multidimensional reactive flows (see e.g. authors papers [3,11]). Used one-dimensional gasdynamics model is two-temperature, two-velocity and is based on Navier–Stokes equations for compressible viscous medium involving thermal conductivity, multicomponent diffusion and chemical transformation according to the reduced kinetic mechanism from [12]. The equations for gaseous phase dynamics together with equations of state can be written as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0 \tag{2}$$

$$\frac{\partial Y_k}{\partial t} + u\frac{\partial Y_k}{\partial x} = \frac{1}{\rho}\frac{\partial}{\partial x}\left(\rho D_k \frac{\partial Y_k}{\partial x}\right) + \left(\frac{\partial Y_k}{\partial t}\right)_{\text{ch}} \tag{3}$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = -\frac{1}{\rho}\left(\frac{\partial p}{\partial x} - \frac{\partial \sigma_{xx}}{\partial x}\right) - \frac{\rho_p}{\rho}\frac{u - u_p}{\tau_{\text{St}}} \tag{4}$$

$$\frac{\partial E}{\partial t} + u\frac{\partial E}{\partial x} = -\frac{1}{\rho}\left(\frac{\partial p u}{\partial x} - \frac{\partial \sigma_{xx} u}{\partial x} - \frac{\partial}{\partial x}\left(\kappa\frac{\partial T}{\partial x}\right) - \rho\sum_k h_k \frac{dY_k}{dt}\right) - \frac{\rho_p}{\rho}\left(u_p\frac{u - u_p}{\tau_{\text{St}}} + c_{P,p}\frac{T - T_p}{\tau_Q}\right) \tag{5}$$

$$p = nRT \tag{6}$$

$$E = \varepsilon + \frac{u^2}{2} \tag{7}$$

$$\sigma_{xx} = \frac{4}{3}\mu\frac{\partial u}{\partial x} \tag{8}$$

where u and u_p are correspondingly gas and particles flow velocities, E is specific total energy of the gaseous phase, σ_{xx} – viscous stress tensor, μ, κ and D_k are correspondingly gaseous molecular viscosity, thermal conductivity and molecular diffusion of the kth species, $n = \sum_k Y_k$ – gaseous molar density, term $\left(\frac{\partial Y_k}{\partial t}\right)_{\text{ch}}$ determines

the changing in the mixture compound due to the chemical transformations in the reaction zone and is calculated from the ordinary differential equations (ODE) system related to the chosen kinetics scheme:

$$\frac{dY_k}{dt} = F(Y_i, T), \quad i = 1, N \tag{9}$$

Variables τ_{St} and τ_Q are characteristic time scales of momentum and heat exchange between gaseous phase and continuum of suspended micro particles. According to Stokes law for spherical particles τ_{St} is calculated as:

$$\tau_{St} = m_p/3\pi\mu d_p \tag{10}$$

Time scale of interphase heat exchange τ_Q is calculated as:

$$\tau_Q = d_p^2 c_{P,p}\rho_{p0}/6\kappa \mathrm{Nu} \tag{11}$$

where Nu is Nusselt number (see e.g. [13]).

The continuum approximation for dispersed phase of suspended microparticles can be written as:

$$\frac{\partial N_p}{\partial t} + \frac{\partial N_p u_p}{\partial x} = 0 \tag{12}$$

$$\frac{\partial u_p}{\partial t} + u_p\frac{\partial u_p}{\partial x} = \frac{u - u_p}{\tau_{St}} \tag{13}$$

$$\frac{\partial T_p}{\partial t} + u_p\frac{\partial T_p}{\partial x} = \frac{T - T_p}{\tau_Q} - \frac{\pi d_p^2}{2}\frac{N_p}{c_{P,p}\rho_{p0}}\left(4\sigma T_p^4 - q_{\mathrm{rad}}\right) \tag{14}$$

where the last term in the right hand part of Eq. (14) is the thermal radiation heat flux absorbed and reemitted by the particles, q_{rad} – radiative heat flux, σ – Stefan–Boltzman constant. Radiative heat transfer was calculated according to the diffusive approximation [14] with assumption that each suspended particle absorbs and re-emits thermal radiation as a black body:

$$\frac{d}{dt}\left(\Lambda\frac{dq_{\mathrm{rad}}}{dt}\right) = -\frac{3}{\Lambda}\left(4\sigma T_p^4 - q_{\mathrm{rad}}\right) \tag{15}$$

During the radiative heating no volatilization effects were taken into account and inactive particles did not change their size and phase state. This assumption is quite acceptable as on the stage prior to ignition the temperature did not exceed value of 1050.0–1100.0 K. Afterward the energy balance is changing mainly by the exothermal reaction of combustion and the phase transitions play almost no role in further evolution of combustion.

A coarse-particle method [15] was used to solve both (2)–(8) and (12)–(14) systems of balance equations. This scheme appears to be rather robust when used to model various kinds of complex hydrodynamic flows. The analysis of this method applied to a large variety of problems, including problems of hydrodynamic instability, have shown that it possesses a high numerical stability, which enables to carry out calculations of shock waves without the aid of artificial viscosity. High stability of the method is achieved by dividing one time-step calculation into three stages. On the first stage, the change of hydrodynamic characteristics on the fixed Eulerian space grid is calculated using the explicit scheme without regarding of mass, momentum and energy transfer. The hydrodynamic variables are transferred through the cell boundaries on the second stage using the values of hydrodynamic characteristics from the first stage. The last, third, stage consists in final calculation of the values of all the parameters for every cell with account of both previous stages. The overall solver is of the second-order accurate, providing high accuracy of the solutions. The utilized version of CPM was thoroughly tested and successfully used for simulation a wide range of problems in the field of transient ignition, combustion and detonation phenomena (see our recent papers [3,11] and papers cited within).

Chemical kinetics ODE system (9) was solved using the Gear method [16]. Radiative heat transfer Eq. (14) was solved using the implicit scheme for each gasdynamical time step. For more complete description of the mathematical model for two-phase reactive gasdynamics and the numerical algorithm one can address to the recent paper [11] which also contains the results of algorithm testing on related problems of gas-particles layer ignition and combustion. According to the validation routines carried out recently in [11] and our previous papers it was obtained that one-dimensional solutions for one- and two-phase flames are in adequate agreement with available experimental data on burning velocities in a wide range of initial conditions (temperature, pressure, mixture composition). As it will be shown below the thermal explosion of stoichiometric hydrogen–oxygen mixture inside the heated gas-particles layer occurs at the characteristic ignition temperature of ~1050–1100 K and at almost constant pressure ~1.0 atm. To reproduce accurately the non-steady evolution of thermal explosion and formation of combustion or detonation wave and exclude artificial numerical solutions it is necessary to resolve reaction zones arising at provided ignition conditions. The most rigid criterion arises in the case of detonation. Detonation initiation demands one to use fine as possible numerical grids resolving well the reaction front propagating through the mixture compressed by the shock able to ignite detonation. The front in this case should be reproduced by a larger amount of computational cells compared with shock wave front smoothened due to the numerical scheme viscosity. According to the carried convergence tests the computational cell size should be not greater than 5.0 μm. Therefore in the present paper we used exactly this resolution reproducing numerically all the regimes considered below.

Thermal explosion of gas-particles layer and possible scenarios of detonation formation

The heating of the gaseous mixture is determined by radiative heat absorption on the particles' surfaces and further heat transfer from these surfaces to the surrounding gas. The rate of uniformity of gas heating is fully determined by the volume fraction and spatial distribution of the particles. During the heating process gaseous mixture expands carrying microparticles away from the heated region. As a result the local concentration of the particles decreases. Further heating continues in the non-uniform medium with a larger mean free path as it changes with spatial concentration of the particles (see Eq. (1)). If the particles layer thickness is large such that rarefaction waves have no time to disturb medium inside the layer before the ignition, the temperature distribution will reproduce the profile of radiative flux decreasing exponentially with the depth ($T(x) \sim \exp(-x/\Lambda)$). In the case of thin layer the rarefaction manage to modify spatial concentration of the particles so the heating becomes almost uniform. Fig. 2 represents the characteristic pattern of the process evolution including the stage of heating and expansion, the stage of thermal explosion inside heated layer and the stage of detonation formation inside the fresh fuel. The data are presented for the layer of initial thickness $L_1 \approx 0.45\Lambda$. The heated medium expands almost symmetrically on the first stage. The thermal explosion (2) aroused inside the heated layer generates detonation wave (5) propagating to the "right" into the cold fresh fuel and fast combustion wave (8) that propagates to the "left" toward the energy source. Locus of the self-sustained detonation and fast flame are shown by three isotherms of 1100.0 K, 2000.0 K and 3000.0 K. At the given heat source power the maximum gas temperature inside gas-particle layer prior to ignition achieves a value of 1050–1100 K. After

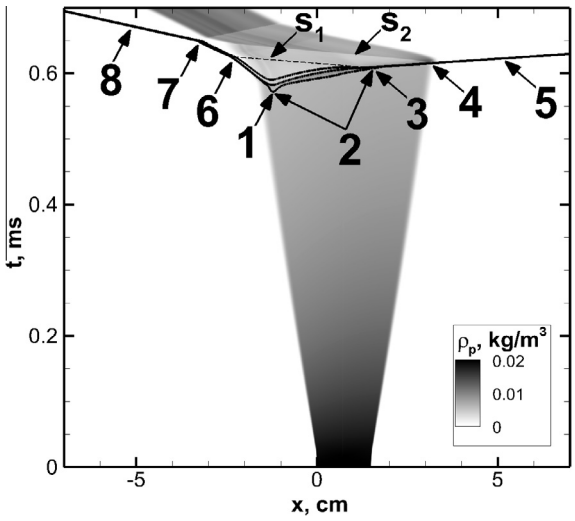

Fig. 2. Gas-particles layer evolution during its radiative heating and thermal explosion. Color palette shows the changes in particles spatial distribution. Solid lines represent isotherms of 1100.0 K, 2000.0 K and 3000.0 K (correspondingly from the bottom line to the top one). 1 – First ignition point, 2 – region of thermal explosion, 3 – point of detonation onset, 4 – detonation enter into fresh fuel, 5 – self-sustained detonation, 6 – left reaction front interaction with retonation wave s_1, 7 – left reaction front interaction with shock wave s_2, 8 – fast flame propagating toward energy source.

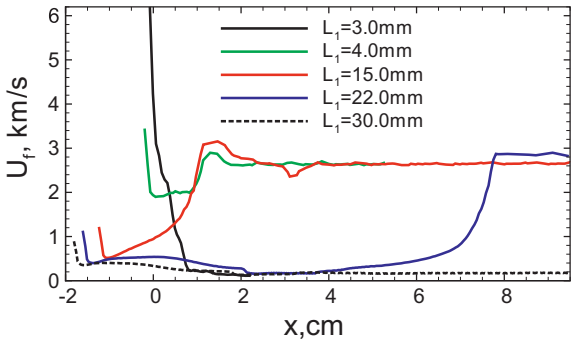

Fig. 3. Speed histories for reaction waves propagating in the direction from the energy source through gas-particles layers of different thicknesses.

ignition the energy of thermal explosion provides temperature rise up to 3100.0 K inside the ignition zone and flame front and up to 3500.0 K inside the detonation front.

In the studied range of particles volume fractions the heating time up to the ignition is longer than the characteristic acoustic time scales ($t_{ign} > \Lambda/c$, where c – local sonic speed). In such a case the ignition arises inside the non-uniformly heated kernel at almost constant pressure. Ignition regimes in such a case correspond to non-stationary thermal explosion basic solution derived by Zel'dovich for the ignition on the temperature gradient [17]. In Fig. 2 isotherms of 1100.0 K, 2000.0 K and 3000.0 K are presented to illustrate the region of thermal explosion evolution. In this region the exothermal reaction proceeds volumetrically during the finite time interval. After the detonation wave is formed all these isotherms coalesce as the exothermal reaction now proceeds inside a relatively narrow zone just behind the shock front that corresponds to the ZND detonation wave structure [18].

According to the regimes' classification proposed in [17] there is a unique correspondence between temperature gradient parameters, peculiarities of thermal explosion evolution and resultant combustion regime. In the presence of temperature gradient (or more generally of reactivity gradient) thermal explosion evolves in the form of so-called spontaneous reaction wave. Spontaneous reaction wave propagates via a series of independent ignitions along temperature gradient with visible speed equal to $U_{sp} = |\mathrm{grad}(\tau_{ind})|^{-1}$ (which can be sufficiently high in case of smooth gradient, as induction period τ_{ind} decreases with temperature rise and asymptotically, when the whole volume is at constant temperature, $U_{sp} \to \infty$). If the visible speed is supersonic the reaction front will be followed by a compression wave. Depending on the peculiarities of chemical kinetics (e.g. non-monotonic dependence $\tau_{ind}(T)$) the spontaneous wave evolution is non-steady and resultant combustion regime may be defined by interactions of transient combustion waves and compression waves generated during the overall process. A detailed analysis of spontaneous wave evolution in the case of hydrogen–oxygen ignition and description of the possible resultant combustion regimes were presented recently in [19].

Consider the regimes of thermal explosion evolution and eventual combustion regimes formed inside the layers of different initial thickness. Fig. 3 shows histories of reaction wave velocities along the x direction for different values of L_1. It represents velocity histories for reaction waves propagating to the "right" (from the energy source). In the case of thin layer a forming temperature distribution is smooth and spontaneous reaction wave turns into a so-called "weak detonation" characterized by higher speed and lower compression rate compared with normal detonation. Such a wave consists of supersonic reaction front followed by the compression wave. Propagating along the temperature gradient the reaction front decelerates and couples with the compression wave that results in detonation formation. However, in the case of the thin layer the heated volume may not be enough for this coupling manage to happen and "weak detonation" will enter the cold fresh fuel that will be not sufficient to ignite self-sustained detonation. Therefore one is able to extract a criterion on minimal layer thickness L_{min} below which no self-sustained detonation formation is possible. According to Fig. 3 a regime without a successive detonation onset in the fresh fuel is realized inside the gas-particles layer of 3.0 mm thickness. In this case spontaneous combustion wave starts with essentially supersonic speed, $U_f(t_{ign}) = 6.2$ km/s, then it is decelerating monotonically while propagating along temperature gradient and during its interaction with contact surface. In this case no stable weak detonation forms inside the layer, and the spontaneous wave degenerates into the combustion wave after entrance into the fresh mixture. In the case of a thicker layer of 4.0 mm thickness a weak detonation establishes, propagates through the layer and forms a detonation inside the fresh fuel after the intersecting the contact surface. The discussion above concerns reaction fronts propagating through the gas-particles layer in the direction from the energy source (1–5 in Fig. 2). In both above mentioned cases the secondary reaction front propagating toward the energy source is weaker and causes formation of deflagration wave instead of detonation. Asymmetry of thermal explosion is fully determined by the non-monotonic temperature distribution inside the heated layer. In the case of an infinitely thin layer the combined effect of heat absorption and rarefaction results in more or less uniform temperature distribution inside layer with rarefaction induced slopes in the regions of contact surfaces. As the layer thickness increases the temperature gradient inside the layer becomes steeper, asymptotically approaching $T(x) \sim \exp(-x/\Lambda)$ distribution. Therefore one can observe a temperature maximum in the vicinity of "left" (near) contact surface. According to this "primal" reaction wave propagates to the "right" along the temperature gradient of spatial length close to the layer thickness while "secondary" reaction wave propagates to the "left" along relatively steep temperature gradient on the spatial scales of contact discontinuity. As layer thickness increases the asymmetry becomes

evident and the role of expansion and continuous radiant heating of gas-particle suspension rises.

In the case of a larger layer thickness and correspondingly steeper temperature gradient the deceleration of spontaneous wave causes its degeneration into the combustion wave. In turn, the compression wave overruns reaction front forming a shock wave. The reaction front accelerates as it consumes the compressed fuel and transforms into the detonation wave (see case L_1 = 15.0 mm in Fig. 3). The mechanism of transient detonation formation is close to that observed in deflagration-to-detonation transition process [20] and immediately after its formation the detonation wave propagates in the "overdriven" regime (alike regime can be also observed in the "SWACER" solution for near-limit direct detonation initiation via spark plug [21]). Overdriven detonation carries higher pressure and temperature and is able to ignite self-sustained detonation in the cold fresh fuel after passing though the contact surface.

With further increase in the layer thickness the formed complex of shock wave followed by the reaction front is unable to initiate detonation and only a fast deflagration wave can be eventually observed. However, there is one more rather unobvious scenario of detonation formation. Shock wave reflects from the contact surface at the far (right) margin of the layer, propagates backward and interacts with the reaction front. The interaction of the reaction front with the shock re-reflected from the near (left) margin is also possible. Additional transfer of the momentum and energy by re-reflected shocks causes reaction front acceleration with sequential transition to detonation. In the most active hydrogen–oxygen mixture the detonation can arise even due to the interaction of accelerating flame with contact surface that takes place in case L_1 = 22.0 mm presented in Fig. 3. This mechanism of transition to detonation due to the shock-to-reaction wave interaction is rather sensitive toward external conditions and should be classified as unstable scenario. Finally, a layer thickness L_{max} exists at which shock attenuates and cannot provide significant acceleration to the flame front. In the absence of reaction front acceleration there is no detonation formation on the scales of gas-particles layer (see e.g. regime taking place in the layer of L_1 = 30.0 mm presented in Fig. 3).

Summing up, it occurs to be possible to ignite self-sustained detonation inside the layers of the thickness between certain limits. Fig. 4 shows zones of considered scenarios of detonation formation depending on the initial layer thickness (L_1) for fixed free mean path Λ while Fig. 5 shows dependence on the initial value of mean free path of radiation (Λ). The detonation arises only in the region between curves 1 and 3 (Fig. 5) in two basic regimes

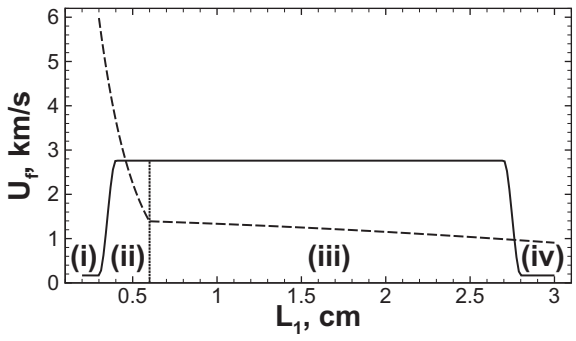

Fig. 4. Initial speed of the spontaneous wave (dashed line) and resultant combustion or detonation wave speed (solid line) for layers of different thicknesses and same particles distribution (Λ = 3.33 cm). (i) Combustion initiation via volumetric thermal explosion, (ii) detonation initiation via thermal explosion, (iii) detonation initiation via transient process, (iv) combustion initiation. Position of margin between regimes (ii) and (iii) (dotted line) is determined by the change in character of spontaneous wave speed dependence.

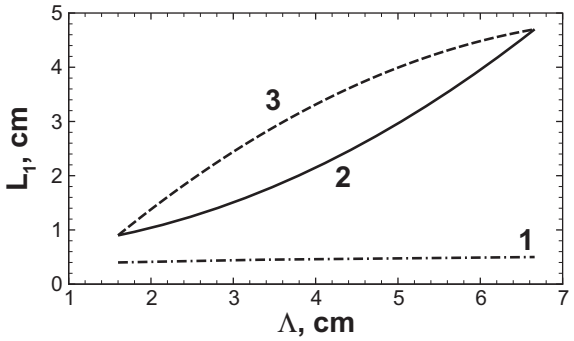

Fig. 5. Calculated criteria of transition between different mechanisms of detonation formation. (1) L_{min} – minimal particles layer thickness sufficient for detonation formation (dash-dotted line), (2) L_{1max} – maximum particles layer thickness providing detonation formation as a result of thermal explosion evolution (solid line), (3) L_{max} – particles layer thickness providing detonation formation (dashed line).

(ii) as a result of volumetric thermal explosion (or "weak detonation") and (iii) as a result of transient combustion regime, involving flame acceleration and its interactions with shock waves and contact surfaces. In the region below curve 2 the detonation arises in full accordance to the non-stationary thermal explosion solution including transient regime involving reaction front acceleration and transition to detonation behind the outrunning shock. In the region above this curve the sufficient role in detonation formation belongs to the secondary shock waves re-reflected from the layer boundaries.

It should be noted that considered regimes of thermal explosion cause detonation triggering in the single direction from the surface of energy source. As discussed above the combustion wave propagating toward the energy source has a deflagrative nature. However, analyzing the evolution of the processes presented in Figs. 2 and 3 one can observe that this secondary reaction front is influenced by the flow of detonation products out from the detonation zone. In the considered case with L_1 = 15.0 mm there are two impulses. First is relatively weak and is generated when the accelerated reaction front transforms into the overdriven detonation. This impulse propagates as a so-called retonation wave (s_1). The second pulse (s_2) is stronger and is generated when the detonation enters the fresh mixture (in case with L_1 = 4.0 mm and weak detonation formation there is only impulse of this second type). As the mixture temperature inside the heated layer is rather high and the induction delay time is correspondingly shorter, one needs less intensive shock wave to sustain steady detonation compared with the shock driving the detonation in the cold fresh mixture. When the detonation in fresh mixture arises the intensity of the combustion products flow increases. Expanding detonation products push the medium in the opposite direction of detonation propagation that can be observed in Fig 2 tracking the particles trajectories. A shock wave arises which overtakes secondary reaction front and accelerates it after their interaction. As a result a fast flame forms with supersonic speed related to the fresh mixture. In the considered one-dimensional case there is no more perturbations in the system able to accelerate this flame further up to the transition to detonation. However in the more realistic two- or three-dimensional case the interactions of the fast flame with the flows forming ahead of its front inside the channel can provide conditions for successive transition to detonation. Such gasdynamical mechanisms of flame acceleration were previously widely discussed in a number of experimental and numerical papers [22–24].

The understanding of detonation onset sensitivity toward mixture composition is crucial for technical applications. Therefore additional calculations were carried out for case of less reactive

hydrogen-air mixture. It was found that for the same conditions considered above the probability of direct detonation initiation in stoichiometric hydrogen–air mixture is sufficiently lower. Thus in the case of $\Lambda = 3.33$ cm self-sustained detonation does not take place at all. In a relatively wide range of L_1 the detonation arises inside the heated layer via the scenario similar to the one presented in Fig. 2 however such detonation wave decays as it intersects the contact surface and enters the cold fresh fuel. The explanation of such an event is following – ignition delay time is sufficiently shorter inside the heated mixture, therefore detonation propagating through the pre-heated mixture is driven by a sufficiently weaker shock wave compared with one necessary to sustain detonation inside the cold fresh fuel. Such a shock is not able to ignite detonation inside the cold fresh fuel in the majority of fuel–air mixtures which are much less reactive then hydrogen–oxygen one. According to this a more complicated additional analysis for less reactive mixtures is needed to understand the applicability of the concept proposed in this paper.

One more non-ideality in problem setup that is significant for the evolution of ignition and detonation formation is non-uniformity in particles spatial distribution. Here such a distribution was modeled as a system of thin particles layers (~0.1–1.0 cm) separated by layers of a pure gaseous mixture. On the stage of radiative heating the outer layers screen the inner layers diminishing the role of rarefaction. As a result the heating up to the ignition temperature occurs faster compared with the case of a single layer. At the same time the maximum of the temperature is located in the central part of the system. For example in the case presented in Fig. 6 only two middle layers occur to be heated up to the ignition temperature (~1100.0 K) prior to ignition. Here reaction wave evolves not in accordance to the spontaneous mechanism but via a combined mechanism involving gasdynamical impact of the already ignited layer on the neighboring one. Shocks emitted out from the ignition kernels transfer momentum and energy triggering faster ignition of the neighboring heated layers. Thus in the case presented in Fig. 6 the remote layers are heated up to the ignition temperature via arriving shock waves that can be registered as the joint growth in particles mass density and temperature. Ignition of every next gas-particles layer occurs in a more compressed medium. The visible speed of the reaction front increases as well as the shock intensity that finally causes transition to detonation. It should be noted that the position of primal ignition kernel in the central part can result in detonation formation in two directions away from and toward the energy source. Finally one can observe particles gathered together by two converging shock waves pushed by detonation products (Fig. 6).

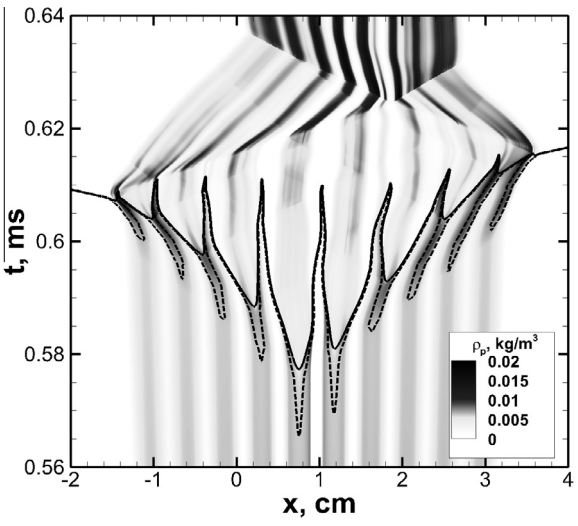

Fig. 6. Particles distribution evolution during the ignition in the multi-layered system of 10 · 1.0 mm gas-particles layers split with 1.0 mm gas layers. Lines represent isotherms of 1100.0 K (dashed) and 2000.0 K (solid).

Here it is useful to notice that observed mechanism of multi-kernel ignition differs from usually accepted one (see e.g. [10]). Usually it is assumed that the basic mechanism responsible for detonation onset in a multi-kernel system is the initial large surface of forming reaction front and the corresponding relatively large burning velocity. In such an approach dynamical interactions between ignition kernels are not considered. But it is not appropriate as the influence of these interactions can be sufficient like in the considered case presented in Fig. 6.

In addition let us also consider the sensitivity toward the choice of particles' sizes and volumetric fraction. It is easy to see that both increasing in the particles' size and particles' number density are able to provide faster heating up to the ignition temperature. First because of increase in inertia. Second due to decrease in mean free path. Massive particles are more resistive toward the flows generated by the expanding heated gas. Due to this massive particles begin to interact with the cold gas after a longer period of time that determines less heat outflow and as a result faster radiative heating of the particles. Smaller mean free path as a result of a larger number density of the particles also causes faster heating as the total heat energy is absorbed inside the smaller spatial region. At first sight the fact of faster heating might increase the stability of the formulated approach. Furthermore as the time of heating is decreased the primal ignition point tends to shift toward the initial position of the near layer margin that provides a high rate of detonation origin localization. However, one should take into account that the temperature equilibrium between radiatively heated particles and gas establishes only during the finite time τ_Q, determined by the relaxation of the gaseous temperature to the particles temperature and by the heat transfer through the gas between neighboring particles. Therefore the temperature equilibrium calculated according to two-temperature model will be possible only if the duration of heating (t_{ign}) is large enough compared with τ_Q. Otherwise one obtains a system consisting of hot particles suspended inside the cold gas. In such a case ignition arises independently in the vicinity of spatially separated particles that is distinct to the above discussed case of non-uniform particles distribution and cannot provide conditions for detonation formation as the reaction fronts evolve inside small kernels ($\sim d_p$) and the dissipation can prevent volumetric thermal explosion with necessary parameters. According to its determination the time scale τ_Q can be estimated as:

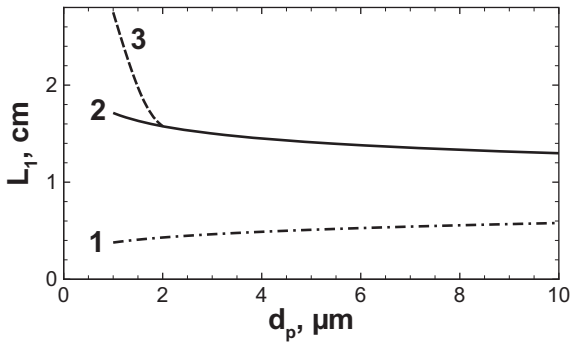

Fig. 7. Calculated criteria of transition between different mechanisms of detonation formation similar to those presented in Fig. 5 but for constant $\Lambda = 3.33$ cm and different particles sizes. (1) L_{min} (dash-dotted line), (2) L_{1max} (solid line), (3) L_{max} (dashed line).

$$\tau_Q = \frac{d_p^2 c_{P,p}\rho_{p0}}{6\kappa \mathrm{Nu}}\frac{\rho_p}{\rho} + \frac{L_0^2 c_{V,g}\rho}{2\kappa} \quad (16)$$

where $\rho_p = \alpha_p\rho_{p0}$ – mass density of the particles phase, $c_{V,g}$ – gas specific heat capacity, L_0 – mean distance between neighboring particles, that can be estimated as $L_0 = \sqrt[3]{m_p/\rho_p}$, m_p – particle mass. For parameters considered above (case of $d_p = 1.0$ μm and $\Lambda = 3.33$ cm) time of inter-phase heat transfer ~0.1 μs while time of heat redistribution between neighboring particles is about 30–40 μs. t_{ign} for this case is about 550 μs (see Fig. 2) that determines successful detonation onset due to the radiative heating. In case of 10.0 μm particles suspended with volumetric fraction providing the same free mean path $\Lambda = 3.33$ cm time of inter-phase heat transfer increases and becomes of the order of ~100.0 μs while time of heat redistribution between neighboring particles decreases and becomes 10–20 μs. The probability of detonation initiation decreases as the calculated time of radiative heating up to the ignition temperature of 1100 K occurs to be of the order or even less than τ_Q. The calculated value of t_{ign} is of the order of ~220 μs when $\tau_Q = 100$–120 μs.

In addition to these peculiarities intrinsic to small scales (~L_0) the large-scale temperature distribution formed in the discussed case is characterized by the steeper temperature gradients because of less smoothening of massive particles layer due to heated gas expansion. Calculated criteria of transition between different mechanisms of thermal explosion for different particles sizes are presented in Fig. 7. One can observe that an increase in particles' size diminishes the range of layer thicknesses corresponding to the successive detonation onset. Besides, in the case of larger particles there is no detonation formation via unstable scenario involving shock-to-reaction wave interactions.

Conclusions

The presented numerical results demonstrate a new concept for controllable (adjusted position and time) direct gaseous detonation initiation via the radiative heating of the inactive microparticles suspended in the combustible mixture. It is shown that the success of detonation initiation depends on the gas-particles layer structure. The layer structure fully determines the ignition kernel parameters (temperature distribution inside the layer prior to ignition) and as a result the regime of thermal explosion evolution. Heating of the single layer of spatially uniformly distributed particles principally can provide a directed detonation wave. The non-uniformities in particles spatial distribution cause principal changes in the regimes of ignition and detonation formation and can cause isotropic propagation of detonation.

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